

ABSTRACT

The ability of a query compound to modulate the biological activity of a receptor in a multicellular organism is predicted on the basis of its interaction with that receptor in the presence of various member of a panel of BioKeys. The BioKeys are ligands, especially peptides or nucleic acids, known to recognize the conformation of the receptor. This interaction data, known as a "fingerprint", is compared to the fingerprints for reference compounds with known biological activities mediated by that receptor.

In the "molecular braille" (MB) embodiment of the present invention, the reference and test fingerprints are based on in vitro (cell-free) assays.

In the "cellular-braille" (CB) embodiment of the present invention, the reference and test fingerprints are based on cellular assays (but not on assays of whole multicellular organisms, or their organs or tissues).